Iterative Solution for Effective Interactions in a System with Non-degenerate Unperturbed Energies

K. Suzuki[a], R. Okamoto[a], P.J. Ellis[b], and T.T.S. Kuo[c]

[a]Department of Physics, Kyushu Institute of Technology, Kitakyushu 804, Japan

[b]School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455

[c]Department of Physics, State University of New York at Stony Brook, Stony Brook, NY 11794

Abstract

We generalize the Lee-Suzuki iteration method for summing the folded diagram series to the case where the unperturbed model-space energies are non-degenerate. A condition is derived for the convergence of the iteration scheme and this depends on the choice of the model space projection operators. Two choices are examined, in the first the projection operators are defined in terms of the unperturbed states and in the second they are defined in terms of the eigenfunctions obtained at each stage of the iteration. As is illustrated by calculations with a simple model, the second procedure gives the better convergence and, by suitable choice of the starting energies, allows the reproduction of any subset of the exact eigenvalues.

PACS number: 21.60.Cs

1 Introduction

In nuclear, atomic and chemical physics it is usually necessary to recast the full many-body problem in the form of an effective interaction acting within a chosen model space for which the eigenvalues can be obtained exactly. Much work has been carried out on this topic, both as regards formal questions and actual calculations, see refs. [1–5] for the nuclear case. The formalism consists of a completely linked perturbation series which contains both non-folded and folded diagrams. For a given set of non-folded diagrams, the folded diagram series can be summed by using either the Krenciglowa-Kuo (KK) technique [6] or the Lee-Suzuki (LS) method [7]. Both these methods employ completely degenerate unperturbed energies for the model space, however their convergence properties are different. The KK approach, when convergent, yields the eigenvalues for those states which have the largest overlap with the chosen model space. On the other hand the LS method reproduces those eigenvalues which lie closest to the chosen unperturbed energy.

Since actual single particle energies in, for example the (sd) or the (pf) shells, are far from degenerate, it is clearly desirable to use a formalism which is not restricted to exact degeneracy. This would allow one to treat the one-body terms as unperturbed energies rather than introducing artificial energy shifts so as to rewrite the problem in degenerate form. Further the KK and LS methods yield only certain of the exact eigenvalues which is not, in general, desirable. This restriction is not present in the exact representation of the complete many-body problem as a series of non-folded and folded diagrams

since this contains information regarding all of the true eigenvalues. Given a model space of dimension d it should be possible to obtain any selection of d eigenvalues from the complete set of true eigenvalues. We shall show that this is indeed possible using the formalism developed in this paper which is expressly designed for non-degenerate unperturbed energies.

The organization of this paper is as follows. In sec. 2 we briefly outline the standard LS formalism and establish notation. The generalization of the LS approach to the non-degenerate case is discussed in sec. 3. Since the solution of the equations requires iteration, we give in sec. 4 a criterion for the convergence of the iteration. In order to assess the present approach and to compare with the KK and LS methods, we need to study a case where the exact results are known, i.e. a model. This is the subject of sec. 5. Our concluding remarks are given in sec. 6.

2 Outline of the Lee-Suzuki Method

In the usual way we write the full Hamiltonian, $H = H_0 + V$, where H_0 is the unperturbed Hamiltonian and V is the perturbation. We use a basis in which H_0 is diagonal and define an operator P which projects the Hilbert space onto the chosen model space of dimension d. The complementary operator Q projects onto the remainder of the Hilbert space, thus $P + Q = 1$, $PQ = 0$. Then it is straightforward to obtain formal expressions for the standard non-Hermitian effective interaction, which we denote here by R. It can be derived by a number of different methods [1, 5, 8] and can be written in various forms.

Here it is convenient to use

$$R = PVP + PVQ\omega ,\tag{1}$$

where the operator ω obeys the equation

$$QVP + QHQ\omega - \omega PHP - \omega PVQ\omega = 0 .\tag{2}$$

Then the model-space eigenvalue equation, yielding d of the true eigenvalues labelled E_p, can be written

$$(PH_0P + R)|\phi_p\rangle = E_p|\phi_p\rangle ,\tag{3}$$

where the model space wave function is the projection of the true wave function on the model space, *i.e.*, $\phi_p = P\Psi_p$.

In this section we consider a system with degenerate unperturbed energies, thus

$$PH_0P = \epsilon_0 P .\tag{4}$$

In this case the equation for ω becomes

$$(\epsilon_0 - QHQ)\omega + \omega(PVP + PVQ\omega) = QVP ,\tag{5}$$

which can be rewritten in the form

$$\omega = \frac{1}{\epsilon_0 - QHQ}QVP - \frac{1}{\epsilon_0 - QHQ}\omega R .\tag{6}$$

Substituting eq. (6) into eq. (1), we have

$$R = \left[1 + PVQ\frac{1}{\epsilon_0 - QHQ}\omega\right]^{-1}\hat{Q}(\epsilon_0) ,\tag{7}$$

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where we have defined the $\hat{Q}$-box according to

$$\hat{Q}(\epsilon_0) = PVP + PVQ\frac{1}{\epsilon_0 - QHQ}QVP \ . \tag{8}$$

The LS method [7] generates the solution of eqs. (6) and (7) by iteration. The nth iteration is obtained from the $(n-1)^{\text{st}}$ iteration by the following equations

$$R_n = \left[P + PVQ\frac{1}{\epsilon_0 - QHQ}\,\omega_{n-1} \right]^{-1} \hat{Q}(\epsilon_0) \ , \tag{9}$$

and

$$\omega_n = \frac{1}{\epsilon_0 - QHQ}QVP - \frac{1}{\epsilon_0 - QHQ}\,\omega_{n-1}R_n \ . \tag{10}$$

Defining $\omega_0 = 0$, the nth iterative solution, $(n > 2)$, is given by

$$R_n = \left[P - \hat{Q}_1 - \hat{Q}_2 R_{n-1} - \cdots - \hat{Q}_{n-1} R_2 R_3 \cdots R_{n-1} \right]^{-1} \hat{Q}$$

$$= \left[P - \hat{Q}_1 - \sum_{m=2}^{n-1} \hat{Q}_m \prod_{k=n-m+1}^{n-1} R_k \right]^{-1} \hat{Q} \ , \tag{11}$$

where $\hat{Q}_m$ for $m = 1, 2, \ldots$ is given by the mth derivative of the $\hat{Q}$-box, namely

$$\hat{Q}_m = (-1)^m PVQ \left(\frac{1}{\epsilon_0 - QHQ} \right)^{m+1} QVP = \frac{1}{m!}\frac{d^m\hat{Q}(\epsilon_0)}{d\epsilon_0^m} \ . \tag{12}$$

The sequence $\{R_1, R_2, \ldots\}$ is generally convergent (see sec. 4) so the solution for the effective interaction corresponds to $R = R_\infty$. The rate of convergence and, indeed, which of the exact eigenvalues are obtained from R_∞ will depend on the unperturbed energy ϵ_0. It is important to realize that this is a parameter at our disposal. Thus the Hamiltonian and eq. (5) are unchanged if we shift ϵ_0 to $\epsilon_0 + \epsilon'$ and compensate for this with a corresponding shift of the perturbation V to $V - \epsilon'P$; the quantity ϵ' is clearly arbitrary and can be used to optimize the convergence of the iteration procedure.

3　The Non-degenerate Case

3.1　General Iterative Solution for Effective Interactions

Let us define projection operators, P_α, which act in the model space and are such that

$$P = \sum_\alpha P_\alpha \qquad \text{and} \qquad P_\alpha P_\beta = \delta_{\alpha\beta} P_\alpha .$$ (13)

It follows that

$$P_\alpha P = P P_\alpha = P_\alpha .$$ (14)

We can then discuss the general situation where the model-space eigenvalues of H_0 are not completely degenerate. As in the degenerate case, we have the freedom to modify the unperturbed P-space Hamiltonian arbitrarily and make a compensating change in the P-space part of the perturbation. Such shifts will affect the convergence of the iteration and will determine which of the exact eigenvalues are finally obtained. Thus we choose

$$PH_0'P = \sum_\alpha \epsilon_\alpha P_\alpha \;\; \text{and} \;\; PV'P = PVP + PH_0P - \sum_\alpha \epsilon_\alpha P_\alpha .$$ (15)

This does not exclude the possibility that some degeneracy is still present, indeed the formalism may be applied to the completely degenerate case in which case one regains the standard LS method of the preceding section.

A general perturbative expansion has been given in ref. [9] for the non-degenerate case within the framework of the $\hat{Q}$-box formalism. Here we wish

to generalize the iterative scheme of sec. 2. To that end we substitute $PH_0'P$ in eq. (15) into eq. (2) and multiply by P_α from the right, yielding

$$QVP_\alpha + QHQ\omega P_\alpha - \epsilon_\alpha \omega P_\alpha - \omega(PV'P + PVQ\omega)P_\alpha = 0 \ , \tag{16}$$

from which it follows that

$$\omega P_\alpha = \frac{1}{\epsilon_\alpha - QHQ}QVP_\alpha - \frac{1}{\epsilon_\alpha - QHQ}\omega RP_\alpha \ . \tag{17}$$

Using eq. (13) and noting that $\omega P \equiv \omega$ we have a generalization of eq. (6) to the non-degenerate case, namely

$$\omega = \sum_\alpha \frac{1}{\epsilon_\alpha - QHQ}QVP_\alpha - \sum_\alpha \frac{1}{\epsilon_\alpha - QHQ}\omega RP_\alpha \ . \tag{18}$$

Multiplying eq. (1) on the right by P_α, using eq. (17) and noting that $R \equiv RP = \sum_\alpha RP_\alpha$, we have a formal solution for R given by

$$R = \sum_\alpha \left[1 + PVQ\frac{1}{\epsilon_\alpha - QHQ}\omega\right]^{-1}\hat{Q}(\epsilon_\alpha)P_\alpha \ , \tag{19}$$

where $\hat{Q}(\epsilon_\alpha)$ is similar to eq. (8), namely

$$\hat{Q}(\epsilon_\alpha) = PV'P + PVQ\frac{1}{\epsilon_\alpha - QHQ}QVP \ . \tag{20}$$

We now set up iterative equations for ω and R. In the most general case the projection operators may vary according to the iteration, i.e. $P_\alpha \to P_\alpha^n$. This means that $\hat{Q} \to \hat{Q}^n$ since it is dependant on the iteration through the quantity $PV'P = PVP + PH_0P - \sum_\alpha \epsilon_\alpha P_\alpha^n$. We can write the iterative equations in the form

$$R_n = \sum_\alpha \left[P + PVQ\frac{1}{\epsilon_\alpha - QHQ}\omega_{n-1}\right]^{-1}\hat{Q}^{n-1}(\epsilon_\alpha)P_\alpha^{n-1} \ , \tag{21}$$

and

$$\omega_n = \sum_\alpha \left[\frac{1}{\epsilon_\alpha - QHQ}QVP_\alpha^{n-1} - \frac{1}{\epsilon_\alpha - QHQ}\omega_{n-1}R_nP_\alpha^{n-1}\right] \ . \tag{22}$$

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This is just the generalization of the LS eqs. (9) and (10) to the non-degenerate case. We define P_α^0 in terms of the basis states of the original unperturbed Hamiltonian, thus

$$P_\alpha^0 = |\alpha\rangle\langle\alpha| \qquad \text{where} \qquad H_0|\alpha\rangle = \epsilon_\alpha|\alpha\rangle \ . \tag{23}$$

Taking $\omega_0 = 0$, we have the sequence

$$R_1 = \sum_\alpha \hat{Q}^0(\epsilon_\alpha)P_\alpha^0 \ , \tag{24}$$

$$R_2 = \sum_\alpha \left[P - \sum_\beta \hat{Q}_1(\epsilon_\alpha, \epsilon_\beta)P_\beta^0 \right]^{-1} \hat{Q}^1(\epsilon_\alpha)P_\alpha^1 \ , \tag{25}$$

$$R_3 = \sum_\alpha \left[P - \sum_\beta \hat{Q}_1(\epsilon_\alpha, \epsilon_\beta)P_\beta^1 - \sum_{\beta\gamma} \hat{Q}_2(\epsilon_\alpha, \epsilon_\beta, \epsilon_\gamma)P_\beta^0 R_2 P_\gamma^1 \right]^{-1} \hat{Q}^2(\epsilon_\alpha)P_\alpha^2, \tag{26}$$

and in general R_n, for $n > 2$, is given by

$$R_n = \sum_\alpha \left[P - \sum_\beta \hat{Q}_1(\epsilon_\alpha, \epsilon_\beta)P_\beta^{n-2} - \sum_{\beta\gamma} \hat{Q}_2(\epsilon_\alpha, \epsilon_\beta, \epsilon_\gamma)P_\beta^{n-3} R_{n-1} P_\gamma^{n-2} \cdots \right.$$

$$\left. - \sum_{\beta\gamma\cdots\lambda\mu} \hat{Q}_{n-1}(\epsilon_\alpha, \epsilon_\beta, \epsilon_\gamma, \cdots \epsilon_\lambda, \epsilon_\mu)P_\beta^0 R_2 P_\gamma^1 R_3 \cdots R_{n-2} P_\lambda^{n-3} R_{n-1} P_\mu^{n-2} \right]^{-1}$$

$$\hat{Q}^{n-1}(\epsilon_\alpha)P_\alpha^{n-1}$$

$$= \sum_\alpha \left[P - \sum_\beta \hat{Q}_1(\epsilon_\alpha, \epsilon_\beta)P_\beta^{n-2} - \sum_{m=2}^{n-1} \sum_{\beta_1\beta_2\cdots\beta_m} \hat{Q}_m(\epsilon_\alpha, \epsilon_{\beta_1}, \cdots, \epsilon_{\beta_m}) \right.$$

$$\left. \times P_{\beta_1}^{n-m-1} \prod_{k=n-m+1}^{n-1} R_k P_{\beta_{k-n+m+1}}^{k-1} \right]^{-1} \hat{Q}^{n-1}(\epsilon_\alpha)P_\alpha^{n-1}. \tag{27}$$

Here we have defined

$$\hat{Q}_1(\epsilon_1, \epsilon_2) = -PVQ\frac{1}{\epsilon_1 - QHQ}\frac{1}{\epsilon_2 - QHQ}QVP$$

$$= \begin{cases} \frac{\hat{Q}(\epsilon_1) - \hat{Q}(\epsilon_2)}{\epsilon_1 - \epsilon_2} & \text{if } \epsilon_1 \neq \epsilon_2 \\ \frac{d\hat{Q}(\epsilon)}{d\epsilon}\Big|_{\epsilon=\epsilon_1} & \text{if } \epsilon_1 = \epsilon_2 \end{cases}, \tag{28}$$

and, in general,

$$\hat{Q}_m(\epsilon_1, \epsilon_2, \cdots, \epsilon_{m+1}) = (-1)^m PVQ \frac{1}{\epsilon_1 - QHQ} \frac{1}{\epsilon_2 - QHQ} \cdots$$
$$\cdots \frac{1}{\epsilon_{m+1} - QHQ} QVP . \quad (29)$$

3.2 Choice of Projection Operator

The simplest choice is to keep P_α fixed at its initial value, namely

$$P_\alpha^n = P_\alpha^0 = |\alpha\rangle\langle\alpha| . \quad (30)$$

This means that $PV'P = PVP$ so that $\hat{Q}^n$ is independant of n and is the same as $\hat{Q}$ of eq. (8). We refer to this as the generalized Lee-Suzuki approach (GLS). We can easily regain the results of sec. 2 in the completely degenerate case where $\epsilon_\alpha = \epsilon_0$ for all α. Thus $\hat{Q}_m(\epsilon_1, \epsilon_2, \cdots, \epsilon_{m+1})$ becomes simply the $\hat{Q}_m$ of eq. (12). This means that the summations in eq. (27) are just of the form $\sum_{\beta_i} P_{\beta_i} = P$ and since $\hat{Q}_m P = \hat{Q}_m$ we return to eq. (11).

The other choice we consider for the projection operators is to write them in terms of the model space wave functions obtained at each iteration. Specifically our n^{th} approximation to the exact eq. (3) is

$$\left(\sum_\alpha \epsilon_\alpha P_\alpha^{n-1} + R_n \right) |\phi_\alpha^n\rangle = E_\alpha^n |\phi_\alpha^n\rangle , \quad (31)$$

where E_α^n is the nth approximation to the true eigenvalue E_α. The vectors $|\phi_\alpha^n\rangle$, being simply the projections of the true wave functions onto the model space, are not orthogonal. However it is well known that their biorthogonal complements $|\tilde{\phi}_\alpha^n\rangle$ can be defined such that $\langle\tilde{\phi}_\alpha^n|\phi_\beta^n\rangle = \delta_{\alpha\beta}$. We then define

$$P_\alpha^n = |\phi_\alpha^n\rangle\langle\tilde{\phi}_\alpha^n| , \quad (32)$$

and it is easily verified that eqs. (13) and (14) are satisfied. It is necessary to specify which ϵ_α is associated with a given P_α in eq. (31). This we do in the obvious way by ordering the unperturbed energies $\epsilon_1 < \epsilon_2 < \cdots < \epsilon_d$ and the approximate energies $E_1^n < E_2^n < \cdots < E_d^n$ and making the association with the corresponding eigenvectors. We refer to this as the generalized Lee-Suzuki method with self-consistent basis (SCGLS). In the completely degenerate case $\sum_\alpha \epsilon_\alpha P_\alpha^n$ becomes $\epsilon_0 \sum_\alpha P_\alpha^n = \epsilon_0 P$ and the approach reverts to the standard LS method by the arguments given before.

3.3   Evaluation of $\hat{Q}_m$

The operator $\hat{Q}_m(\epsilon_1, \epsilon_2, \cdots, \epsilon_{m+1})$ is the basic element needed to construct the effective interaction for the non-degenerate case and it can be expressed as a linear combination of the standard $\hat{Q}$-boxes according to

$$\hat{Q}_m(\epsilon_1, \epsilon_2, \cdots, \epsilon_{m+1}) = \sum_{k=1}^{m+1} C_k(\epsilon_1, \epsilon_2, \cdots, \epsilon_{m+1}) \hat{Q}(\epsilon_k) , \tag{33}$$

where

$$C_k(\epsilon_1, \epsilon_2, \cdots, \epsilon_{m+1}) = \left[(\epsilon_k - \epsilon_1)(\epsilon_k - \epsilon_2) \cdots (\epsilon_k - \epsilon_{k-1})(\epsilon_k - \epsilon_{k+1}) \cdots \right.$$
$$\left. \cdots (\epsilon_k - \epsilon_{m+1}) \right]^{-1} . \tag{34}$$

For the derivation of eq. (33) we have used the equality

$$\left[(\epsilon_1 - QHQ) \cdots (\epsilon_{m+1} - QHQ) \right]^{-1} = \sum_{k=1}^{m+1} (-1)^m \frac{C_k(\epsilon_1, \epsilon_2, \cdots, \epsilon_{m+1})}{\epsilon_k - QHQ}, \tag{35}$$

which is easily proved by induction. It should be noted that the term $PV'P$ in the $\hat{Q}$-box (eq. (20)) gives no contribution to eq. (33) because of the

relation

$$\sum_{k=1}^{m+1} C_k(\epsilon_1, \epsilon_2, \cdots, \epsilon_{m+1}) = 0 \ , \tag{36}$$

which can be proved directly from eq. (34).

So far we have implicitly assumed that the energies $(\epsilon_1, \epsilon_2, \cdots, \epsilon_{m+1})$ are all different. However in carrying out the summations we shall need to consider the case where two or more of the energies refer to the same state and there may also be some degeneracy present. Suppose, for instance, that $\epsilon_1 = \epsilon_2$ so that the formal limit $\epsilon_1 \to \epsilon_2$ leads to the derivative as in eq. (28). This is actually evaluated by calculating $\hat{Q}_1(\epsilon_1, \epsilon_1 + \delta)$ or, in general, $\hat{Q}_m(\epsilon_1, \epsilon_1 + \delta, \epsilon_3, \cdots, \epsilon_{m+1})$, where δ is small in comparison to ϵ_1. Similarly if $\epsilon_1 = \epsilon_2 = \epsilon_3$, we would use $\hat{Q}_m(\epsilon_1 - \delta, \epsilon_1, \epsilon_1 + \delta, \epsilon_4, \cdots, \epsilon_{m+1})$, and so on. Thus the fundamental quantity we need is $\hat{Q}(\epsilon_k + p\delta)$, where $p = 0, \pm 1, \pm 2, \ldots$ and this only differs from the degenerate case in that here more than one value of ϵ_k needs to be considered. Thus in applying eqs. (33) and (34) any degeneracy should be broken by a small amount so that the appropriate derivative is implicitly evaluated.

4 Convergence of the Iterative Solution

We now discuss the convergence condition for the generalized LS iteration scheme. Let $\delta\omega_{n-1}$ and $\delta\omega_n$ be the deviations from the exact solution ω of eq. (18) in the $(n-1)^{\text{st}}$ and n^{th} iterations respectively. Thus, by definition,

$$\omega_{n-1} = \omega + \delta\omega_{n-1} \ , \tag{37}$$

$$\omega_n = \omega + \delta\omega_n \ . \tag{38}$$

We first discuss the case where the projection operator is fixed, *i.e.*, $P_\alpha^n = P_\alpha^0$. Now setting $R_n = R + \delta R_n$, we find from eq. (1) that $\delta R_n = PVQ\delta\omega_n$. Then to first order in $\delta\omega$, using eq. (22), we have

$$[\epsilon_\alpha - (QHQ - \omega PVQ)]\,\delta\omega_n P_\alpha^0 = -\delta\omega_{n-1}RP_\alpha^0 \ . \tag{39}$$

Now the term $(QHQ - \omega PVQ)$ is the Q-space effective Hamiltonian [7]. The eigenvalue equation for this case can be written in the form

$$\langle\psi_q|(QHQ - \omega PVQ) = E_q\langle\psi_q| \ . \tag{40}$$

The eigenvalues E_q above and E_p in eq. (3) agree with two of the exact eigenvalues of the Hamiltonian H. Now dividing eq. (39) by the operator in square brackets on the left and multiplying by $\langle\psi_q|$ on the left and $|\phi_p\rangle$ on the right, we obtain

$$\langle\psi_q|\delta\omega_n P_\alpha^0|\phi_p\rangle = \langle\psi_q|\delta\omega_{n-1}RP_\alpha^0|\phi_p\rangle(E_q - \epsilon_\alpha)^{-1} \ . \tag{41}$$

This can be simplified by using $|\tilde{\phi}\rangle$, the biorthogonal complement to $|\phi\rangle$, and inserting $\sum_{p'}|\phi_{p'}\rangle\langle\tilde{\phi}_{p'}| = \mathbf{1}$ since

$$\langle\tilde{\phi}_{p'}|RP_\alpha^0 = (E_{p'} - \epsilon_\alpha)\langle\tilde{\phi}_{p'}|P_\alpha^0 \ . \tag{42}$$

Performing these manipulations and summing over α in eq. (41), we finally obtain

$$\langle\psi_q|\delta\omega_n|\phi_p\rangle = \sum_{p'}\langle\psi_q|\delta\omega_{n-1}|\phi_{p'}\rangle Z_{p'p}^q \ , \tag{43}$$

where we have defined

$$Z_{p'p}^q = \sum_\alpha \left(\frac{\epsilon_\alpha - E_{p'}}{\epsilon_\alpha - E_q}\right)\left\langle\tilde{\phi}_{p'}\left|P_\alpha^0\right|\phi_p\right\rangle \ . \tag{44}$$

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It is useful to write eq. (43) in an obvious matrix notation as

$$\delta\boldsymbol{\omega}_n = \delta\boldsymbol{\omega}_{n-1} \cdot \mathbf{Z} \ . \tag{45}$$

Then in order that the iteration be convergent it is necessary that the norm $\parallel \delta\boldsymbol{\omega}_n \parallel$ be smaller than $\parallel \delta\boldsymbol{\omega}_{n-1} \parallel$ for n greater than some integer N. This means that a sufficient condition for convergence is

$$\parallel \mathbf{Z} \parallel < 1 \ . \tag{46}$$

Here we employ the Hilbert, or spectrum, norm which is defined for an arbitary matrix $\mathbf{X}$ as $\parallel \mathbf{X} \parallel = \max\sqrt{\lambda_i}$, where λ_i are the eigenvalues of the matrix $\mathbf{X}^\dagger\mathbf{X}$. In the completely degenerate case we see that eqs. (44) and (46) reduce immediately to the LS convergence condition

$$\left| \frac{\epsilon_0 - E_p}{\epsilon_0 - E_q} \right| < 1 \ . \tag{47}$$

Thus eq. (46) represents the generalization of the LS condition to the case of a non-degenerate P-space.

The convergence that is obtained will depend on the choice of projection operator. In the GLS case the condition (46) may be quite complicated, since eq. (44) involves $\left\langle \tilde{\phi}_{p'} \,|P_\alpha^0|\, \phi_p \right\rangle = \left\langle \tilde{\phi}_{p'} \,|\alpha\rangle\langle\alpha|\, \phi_p \right\rangle$. However, if the states that we wish to obtain, $|\phi_p\rangle$, lie largely within the model space the non-Hermiticity of the effective interaction will be small (see the discussion in ref. [10]) and $|\tilde{\phi}_p\rangle$ will not differ greatly from $|\phi_p\rangle$. Further if a given state p contains a large component of $|\alpha\rangle$ we can expect $\mathbf{Z}$ to be close to a diagonal matrix. Then the convergence condition (46) should be satisfied if the unperturbed energy ϵ_α is close to E_p, but distant from the Q-space eigenvalues E_q.

We next discuss the convergence condition for the SCGLS approach. In this case we have to consider the deviation δP_α^n of the projection operator defined as

$$\delta P_\alpha^n = P_\alpha^n - P_\alpha^\infty , \qquad (48)$$

with

$$P_\alpha^\infty = |\phi_\alpha\rangle\langle\tilde{\phi}_\alpha| , \qquad (49)$$

where $|\phi_\alpha\rangle$ is the exact eigenstate in eq. (3). Since R_n in eq. (21) can be written as

$$
\begin{aligned}
R_n &= PV'^{(n-1)}P + PVQ\omega_n \\
&= PVP + PH_0P - \sum_\alpha \epsilon_\alpha P_\alpha^{n-1} + PVQ\omega_n ,
\end{aligned}
\qquad (50)
$$

the deviation δR_n is given by

$$\delta R_n = PVQ\delta\omega_n - \sum_\alpha \epsilon_\alpha \delta P_\alpha^{n-1} . \qquad (51)$$

Substituting eqs. (37), (38) and (51) into eq. (22), we see that, to first order, the terms with the deviation δP_α^{n-1} are all canceled and we have

$$[\epsilon_\alpha - (QHQ - \omega PVQ)]\delta\omega_n P_\alpha^\infty = -\delta\omega_{n-1} R P_\alpha^\infty , \qquad (52)$$

which is just the equation obtained by replacing P_α^0 by P_α^∞ in eq. (39). Directly from eq. (52) or by replacing P_α^0 by P_α^∞ in eq. (44), we obtain the matrix $Z_{pp'}^q$ as

$$Z_{pp'}^q = \left(\frac{\epsilon_p - E_p}{\epsilon_p - E_q}\right)\delta_{pp'} . \qquad (53)$$

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We finally may say that in order that $\| \mathbf{Z} \| < 1$ the following condition must be satisfied:

$$\| \mathbf{Z} \| = \max \left| \frac{\epsilon_p - E_p}{\epsilon_p - E_q} \right| < 1, \quad p = 1, 2, \dots, d, \quad q = 1, 2, \dots \quad . \tag{54}$$

The above condition is satisfied if and only if the d eigenvalues E_p correspond to those true eigenvalues which lie nearest to the unperturbed energies ϵ_p with $p = 1, 2, ..., d$.

The magnitude of $\|\mathbf{Z}\|$ is equal to unity at points where $\epsilon_p = \frac{1}{2}(E_p + E_q)$, *i.e.*, one of the unperturbed energies is exactly halfway between a P-space and a Q-space eigenvalue. Apart from these points eq. (54) is obeyed, so that this iteration scheme will converge to those eigenstates whose eigenvalues lie nearest to the unperturbed energies ϵ_p.

5   Test Calculations

In order to obtain some assessment of the GLS and SCGLS methods, as well as to compare with the KK and LS methods, we need to study a model for which exact results are readily obtained. The model we shall use is a slightly modified version of one which was introduced many years ago by Hoffmann *et al.* [11] in order to study the intruder state problem. The Hamiltonian is taken to be $H = H_0 + V$, where the unperturbed Hamiltonian matrix is

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$H_0 = \mathrm{diag}(1, 1, 3, 9)$ and the perturbation V is given by

$$
V = \begin{pmatrix}
0 & 5x & -5x & 5x \\
5x & 25x & 5x & -8x \\
-5x & 5x & -5x & x \\
5x & -8x & x & -5x
\end{pmatrix},
$$

where x is a parameter that we shall vary. Obviously the eigenvalue problem for this model Hamiltonian can easily be solved.

We shall take the lowest two states of H_0 to be our model space. Our main concern is then to see whether an effective interaction acting in this model space is able to reproduce any pair of exact eigenvalues. In tables 1 and 2 we show results obtained for $x = 0.05$ and 0.20. Physically these cases differ in that for $x = 0.05$ the model space states dominate the eigenvectors of the first and second states, whereas for $x = 0.20$ they dominate the first and third eigenvectors, *i.e.*, increasing the value of x causes a "level crossing" to take place. Using the SCGLS method we show results obtained with various choices for the ϵ_α of eq. (15). We see that as the unperturbed energies change the solutions converge to different pairs of eigenvalues. As predicted in sec. 4, the SCGLS yields the eigenvalues which are nearest to the unperturbed energies. The convergence rates are reasonable in all cases, with accuracy to four decimal places obtained in at most 12 iterations and usually many fewer are required. By adjusting the ϵ_α we are able to reproduce any pair of exact eigenvalues, regardless of the order of the eigenvalues or the magnitude of the P-space overlap of the eigenvectors.

We have also carried out calculations with the GLS method where the projection operators are defined in terms of the unperturbed eigenfunctions

and do not vary with iteration. For $x = 0.20$ we were able to reproduce all pairs of eigenvalues as with the SCGLS, however for $x = 0.05$ we were not able to obtain convergence for three of the combinations. These were (E_1, E_4), (E_2, E_4) and (E_3, E_4). All of them involve state 4 which has a very small overlap with the model space and the quantity Z in eq. (44) depends on the overlaps $\langle \tilde{\phi}_{p'} | \alpha \rangle$ and $\langle \alpha | \phi_p \rangle$ as well as the energy differences $(\epsilon_\alpha - E_{p'})$ and $(\epsilon_\alpha - E_q)$. Therefore it is possible to have $\| \mathbf{Z} \| > 1$, implying no convergence, even though $|(\epsilon_\alpha - E_{p'})/(\epsilon_\alpha - E_q)| < 1$.

We now turn to a comparison of the different iteration methods– KK, LS, GLS, SCGLS. Briefly in the KK method [6] the effective interaction in the nth step is given by

$$R_n = \sum_k \hat{Q}(E_k^{n-1}) |\phi_k^{n-1}\rangle \langle \tilde{\phi}_k^{n-1}| \,, \tag{55}$$

where

$$(PH_0P + R_{n-1})|\phi_k^{n-1}\rangle = E_k^{n-1}|\phi_k^{n-1}\rangle \,. \tag{56}$$

This iterative process sums the folded diagrams to all orders and, if it is convergent, the states with maximium P-space overlap are obtained. For $x = 0.05$ the two lowest states are the ones with maximum P-space overlap and for this case we can compare the four methods. In order to make the comparison we introduce a measure of the deviation of the calculated eigenvalues from the exact results,

$$\Delta_n = \left[\sum_k \left(E_k^n - E_k^{\text{exact}} \right)^2 \right]^{\frac{1}{2}} \,. \tag{57}$$

We plot Δ_n versus the number of iterations n in fig.1. Here we have taken $\epsilon_1 = 1.0$ and $\epsilon_2 = 2.0$ for the GLS and SCGLS and a degenerate energy of

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$\epsilon_0 = 1.5$ for LS and $\epsilon_0 = 1.0$ for KK. Of course all methods converge, but the SCGLS and KK techniques show the fastest convergence. Thus it appears that the use of a self-consistent projection operator yields the most rapid convergence. As another example, we take $x = 0.20$ and reproduce the first and third eigenvalues, which are the ones with maximum P-space overlap, so that the KK, GLS and SCGLS methods can be compared. Taking $\epsilon_0 = 1.0$ for KK and $\epsilon_1 = 0.0, \epsilon_2 = 5.5$ for GLS and SCGLS, we obtain the results in fig. 2. The convergence of the SCGLS method is markedly better than for the other cases. In particular the GLS is rather slowly convergent and shows an oscillatory behavior, although it does ultimately yield an accurate answer. In fig. 3 we make a comparison between LS, GLS and SCGLS at this value of x (using $\epsilon_0 = 4.0$ for LS and $\epsilon_1 = 2.5, \epsilon_2 = 5.5$ for the other cases). These methods converge to the second and third eigenvalues because these lie closest to the unperturbed energies. Here the GLS and SCGLS show a better rate of convergence than the standard LS method, with the SCGLS giving the most rapid rate.

Finally it is of interest to examine the starting energy dependance of the SCGLS method. We show in fig. 4 the effect of varying ϵ_2 while keeping $\epsilon_1 = 0.0$ for $x = 0.20$. The calculations then yield the ground-state energy and either the second or third or fourth eigenvalue depending on ϵ_2. The solid curve in fig. 4 gives the minimum number of iterations, $n_{\min}$, required for $\Delta_n < 10^{-4}$. The convergence is good except at the points where $\epsilon_2 = \frac{1}{2}(E_2 + E_3) = 4.11$ and $\epsilon_2 = \frac{1}{2}(E_3 + E_4) = 7.29$, since here $\| \mathbf{Z} \| = 1$. This is in agreement with the discussion of sec. 4, which suggests that the error in the eigenvalue is proportional to $\|\mathbf{Z}\|^n$, in which case $n_{\min} = c / \log_{10} \|\mathbf{Z}\|$. We

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have plotted this quantity as the dashed curve in fig. 4, choosing the constant c to be -5 and calculating $\parallel \mathbf{Z} \parallel$ with the Q-space eigenstate nearest to ϵ_2. As can be seen the dashed curve agrees very well with the exact result.

6   Concluding Remarks

We have derived an iteration method (GLS) for effective interactions as a generalization of the Lee-Suzuki method so that one can apply it to a system with arbitrary non-degenerate unperturbed energies. It has been proved that the iterative solution can be constructed in the framework of the $\hat{Q}$-box formalism of Kuo *et al.* [3,5] in spite of the non-degeneracy of the unperturbed energies. The convergence in the GLS method depends on the overlaps of the exact P-space eigenstates and the unperturbed states. If the overlaps are small, the GLS approach does not always converge.

The GLS method has further been generalized so that different projection operators can be used in each step of iteration. It has been shown that if we construct the projection operators using the P-space eigenstates determined self-consistently at each iteration step, the convergence is governed only by energy ratios of the differences between true and unperturbed energies and there is, in general, a unique way of distributing the true eigenvalues between the sets E_p and E_q, where E_p denotes the eigenvalues obtained from the P-space eigenvalue equation. This implies that, by appropriate choice of the unperturbed energies, the d eigenvalues obtained from the effective interaction can be tuned to generate any subset of the true eigenvalues. We have verified this theoretical prediction in the model calculations. We have

observed some divergent cases for the GLS, but the use of self-consistent projection operators in the SCGLS renders the iterations convergent. It also accelerates the convergence compared to the usual L-S method.

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Table 1. Convergence of the eigenvalues obtained with the SCGLS method for the model Hamiltonian with $x = 0.05$

| ϵ_1 | ϵ_2 | Number of iterations | | | | | Exact |
		2	4	6	8	10	eigenvalues
1.0	2.0	0.8915	c	c	c	c	E_1
		2.2177	2.2158	c	c	c	E_2
1.0	3.0	0.8966	0.8904	c	c	c	E_1
		2.6998	2.8553	2.8619	c	c	E_3
1.0	9.0	0.9570	0.8900	0.8904	c	c	E_1
		6.8904	8.7779	c	c	c	E_4
2.0	3.0	0.8681	0.5324	2.5126	2.2268	2.2161*	E_2
		2.7209	2.8541	2.8466	2.8621	c	E_3
2.0	9.0	0.9677	1.2027	2.0943	2.2106	2.2155**	E_2
		6.8689	8.7827	8.7816	c	c	E_4
3.0	9.0	1.6722	3.6832	2.8731	2.8625	c	E_3
		7.6619	8.7861	c	c	c	E_4

The notation c indicates convergence to four decimal places. The exact eigenvalues here are $E_1 = 0.8905$, $E_2 = 2.2157$, $E_3 = 2.8622$ and $E_4 = 8.7817$ and the overlaps of the exact eigenfunctions with the model space are 0.973, 0.902, 0.121 and 0.004 respectively.

*Convergence to four decimal places is obtained after 12 iterations.

**Convergence to four decimal places is obtained after 11 iterations.

Table 2. Convergence of the eigenvalues obtained with the SCGLS method for the model Hamiltonian with $x = 0.20$

ϵ_1	ϵ_2	Number of iterations				Exact eigenvalues
		2	4	6	8	
0.0	2.5	-3.0221	-0.2385	c	c	E_1
		4.9933	2.5150	2.5793	c	E_2
0.0	5.5	-0.1608	c	c	c	E_1
		5.6553	c	c	c	E_3
0.0	9.0	-0.1095	-0.1495	c	c	E_1
		8.8437	c	c	c	E_4
2.5	5.5	2.0849	2.5784	c	c	E_2
		5.4309	c	c	c	E_3
2.5	9.0	2.5823	c	c	c	E_2
		8.9173	c	c	c	E_4
5.5	9.0	1.4692	6.3648	5.6463	c	E_3
		8.9215	8.9254	c	c	E_4

The notation c indicates convergence to four decimal places. The exact eigenvalues here are $E_1 = -0.1496$, $E_2 = 2.5794$, $E_3 = 5.6451$ and $E_4 = 8.9251$ and the overlap of the exact eigenfunctions with the model space are 0.715, 0.295, 0.759 and 0.231 respectively.

Figure Captions

Figure 1. The error in the calculated eigenvalues as a function of the number of iterations. Smooth curves are drawn through the points to guide the eye. The curves are labelled by the method employed to solve the model Hamiltonian problem with $x = 0.05$.

Figure 2. As for fig. 1, but with $x = 0.20$. Here the calculations are converging to the first and third eigenvalues.

Figure 3. As for fig. 1, but with $x = 0.20$. Here the calculations are converging to the second and third eigenvalues.

Figure 4. Number of iterations required for an accuracy of one part in 10^4 as a function of the unperturbed energy, ϵ_2, with $x = 0.20$. The full curve is obtained with the SCGLS method and the dashed curve gives the results expected from the convergence analysis, namely $-5/\log_{10} \| \mathbf{Z} \|$.